Thermodynamic fermion-boson symmetry in harmonic oscillator potentials

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Abstract

A remarkable thermodynamic fermion-boson symmetry is found for the canonical ensemble of ideal quantum gases in harmonic oscillator potentials of odd dimensions. The bosonic partition function is related to the fermionic one extended to negative temperatures, and vice versa.

PACS: 05.30.-d; 05.30.Ch; 05.30.Fk; 05.30.Jp

Keywords: Quantum statistics; Canonical ensemble; Finite Fermi and Bose systems

1   Introduction and summary

Finite quantum gases of identical fermions or bosons contained in harmonic oscillator potentials are currently of great interest. The recent motivation stems from the investigation of alkali atoms (bosons) in magnetic traps and the observation of Bose-Einstein condensation, see e.g. [1–3]. On the fermionic side nuclei and their low temperature behaviour are investigated, for instance in [4,5]. If these systems are either only weekly interacting or close to the ground state, they may be considered as an ideal gas of (quasi-) particles confined by a harmonic oscillator potential.

For these finite ideal quantum gases simple expressions, e.g. for the partition function of the canonical ensemble, could not be found up to now, but recursion relations could be derived [6] and used successfully [7–11].

In this article we report that a closer inspection of the canonical partition function uncovers a surprising symmetry property which connects fermions and bosons.

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Fermionic and bosonic N-body partition functions are connected via analytic continuation to negative temperatures. Thermodynamic mean values for the bosonic systems can be easily evaluated knowing the fermionic results and vice versa. Especially for fermions this procedure removes the well-known sign problem because the bosonic partition function does not suffer from alternating signs.

2   Symmetries of the partition function

We consider N identical particles subject to a single-particle Hamiltonian in the canonical ensemble. The partition function Z_N can be recursively built starting with the single-particle partition function [6]

$$Z_N^{\pm}(\beta) = \frac{1}{N} \sum_{n=1}^{N} (\pm 1)^{n+1} \, Z_1(n\beta) \, Z_{N-n}^{\pm}(\beta) \,, \quad Z_0(\beta) = 1 \,, \; \beta = \frac{1}{k_B T} \,, \quad (1)$$

where the upper sign in the sum stands for bosons and the lower sign for fermions. For the case of a three-dimensional harmonic oscillator potential the single-particle partition function is

$$Z_1(\beta) = \left[\frac{\exp\left(-\beta \frac{\hbar \omega}{2}\right)}{1 - \exp(-\beta \hbar \omega)} \right]^3 . \quad (2)$$

Introducing the abbreviation

$$y = \exp(-\beta \hbar \omega) \quad (3)$$

we redefine the partition functions to depend on y, e.g.

$$Z_1(y) = \frac{y^{\frac{3}{2}}}{(1-y)^3} \,. \quad (4)$$

The recursion formula (1) then reads

$$Z_N^{\pm}(y) = \frac{1}{N} \sum_{n=1}^{N} (\pm 1)^{n+1} \, Z_1(y^n) \, Z_{N-n}^{\pm}(y) \,. \quad (5)$$

The partition functions $Z_N^{\pm}$ are rational functions of y and can be split into factors [7,8]

$$Z_N^{\pm}(y) = \frac{y^{\frac{3N}{2}}}{\prod_{j=1}^{N}(1-y^j)^3} \, P_N^{\pm}(y) \tag{6}$$

with $P_N^{\pm}(y)$ being polynomials in y. Obviously this leads to a recursion formula for the polynomials $P_N^{\pm}$

$$P_N^{\pm}(y) = \frac{1}{N} \sum_{n=1}^{N} (\pm 1)^{n+1} \frac{\prod_{j=N-n+1}^{N}(1-y^j)^3}{(1-y^n)^3} \, P_{N-n}^{\pm}(y) \,, \tag{7}$$

where $P_0^{\pm}(y) = 1$ and $P_1^{\pm}(y) = 1$. This is already a useful result since for numerical evaluation recursion formula (7) behaves better.

A closer look at these polynomials opens new insight into fermion-boson symmetry. Consider for example $N = 3$:

$$P_3^{+}(y) = 1 + 3y^2 + 7y^3 + 6y^4 + 6y^5 + 10y^6 + 3y^7 \tag{8}$$
$$P_3^{-}(y) = y^2 \left(3 + 10y + 6y^2 + 6y^3 + 7y^4 + 3y^5 + 1y^7\right) \,.$$

It seems surprising that the coefficients appear in reverse order comparing one polynomial with the other. This is not mere coincidence, but the following theorem holds

$$P_N^{-}(y) = y^{\frac{3}{2}N(N-1)} \, P_N^{+}\left(\frac{1}{y}\right) \,, \tag{9}$$

which can be proven by induction or with the help of an explicit representation as done below. The property of the bosonic and fermionic polynomials leads to a relation between fermionic and bosonic partition functions which is

$$Z_N^{+}(y) = (-1)^N Z_N^{-}\left(\frac{1}{y}\right) \,. \tag{10}$$

Using the usual dependence on the inverse temperature β this property expresses itself as

$$Z_N^{+}(\beta) = (-1)^N Z_N^{-}(-\beta) \,, \tag{11}$$

where the partition function with the negative argument has to be understood as the analytic continuation into the region of $y = \exp(-\beta\hbar\omega) > 1$. In thermodynamic mean values like mean energy or specific heat this symmetry also shows up

$$E_N^{+}(\beta) = -E_N^{-}(-\beta) \quad , \qquad C_N^{+}(\beta) = C_N^{-}(-\beta) \,. \tag{12}$$

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A straight forward application of the above result is to calculate fermionic partition functions and mean values by evaluating the respective bosonic ones at negative temperatures and thereby to avoid the sign problem.

More generally this property is related to the fact that the single-particle partition function has an analytic continuation to the whole β-axis where it is an odd function, $Z_1(-\beta) = -Z_1(\beta)$. Then $Z_N^\pm$ can be analytically extended in the same way and it satisfies eq. (11). We prove this relation rewriting the explicit representation of $Z_N^\pm(\beta)$ as it is given in eq. (8) of ref. [11] in the form

$$Z_N^\pm = (\pm 1)^N \sum_{k=0}^{N-1} \sum_{0<n_1<\cdots<n_k<N} (\pm 1)^{k+1} \frac{\prod_{i=0}^k Z_1\left((n_{i+1} - n_i)\beta\right)}{\prod_{j=1}^k n_j} \,, \tag{13}$$

where we understand $n_0 = 0$ and $n_{k+1} = N$ in the upper product. If β is replaced by $-\beta$ we obtain $(k+1)$ minus signs in the upper product, which either cancel the factor $(-1)^{k+1}$ in the fermionic case or introduce it in the bosonic one and thereby transform the fermionic partition function into the bosonic one or vice versa.

This theorem shows that the fermion-boson symmetry depends only on the oddness of Z_1 and not on the form of the single-particle Hamiltonian. But the harmonic oscillator potentials for odd space dimensions are the only examples we know, where this condition holds.

3 Properties of the polynomials

In order to study the thermodynamics of ideal quantum gases in harmonic oscillator potentials one would like to know more about the polynomials $P_N^\pm$ defined by (6). Using the explicit representation of the partition function (13) one derives

$$P_N^\pm(y) = (\pm 1)^N \prod_{l=1}^N (1 - y^l)^3 \tag{14}$$

$$\times \sum_{k=0}^{N-1} \sum_{0<n_1<\cdots<n_k<N} (\pm 1)^{k+1} \frac{1}{\prod_{j=1}^k n_j \ \prod_{i=0}^k \left(1 - y^{n_{i+1}-n_i}\right)^3} \,.$$

Note, that $P_N^\pm$, although looking like a rational function, is actually a polynomial since $\prod_{i=0}^k \left(1 - y^{n_{i+1}-n_i}\right)^3$ divides $\prod_{l=1}^N (1 - y^l)^3$.

In the following we have to distinguish between properties of $P_N^\pm$, which can be mathematically proven and those which are only established by numerical evidence, i.e. usually checked with MATHEMATICA for several N. For simplicity

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we are considering only bosonic polynomials now, the respective fermionic ones can be obtained by transformation.

The following belongs to the second class (numerical evidence). The coefficients $p_n^{(N)}$ of the polynomials

$$P_N^+(y) = \sum_{n=0}^{L(N)} p_n^{(N)} \, y^n \tag{15}$$

are non-negative and, for $n > 0$ and $N > 4$, monotonically increasing until a maximum is reached and then monotonically decreasing. The degree $L(N)$ satisfies

$$L(N) \leq \frac{1}{2} \left(3N^2 - 7N + 10\right) . \tag{16}$$

The first $N+1$ coefficients $p_n^{(N)}$ are independent of N. They form an approximately exponentially increasing sequence

$$1, 0, 3, 7, 18, 39, 99, 213, 492, 1056, \ldots . \tag{17}$$

For the independence of the first $N/2$ coefficients we know a mathematically exact proof, for the others we have numerical evidence.

Several identities hold for the polynomials, e.g.

$$P_N(1) = (N!)^2 \tag{18}$$
$$P_N'(1) = \frac{3}{4} N(N-1)(N!)^2$$
$$P_N''(1) = \frac{1}{48}(27N^2 - 23N - 8)N(N-1)(N!)^2$$
$$P_N'''(1) = \frac{1}{64}(27N^4 - 42N^3 - 9N^2 + 16N - 20)N(N-1)(N!)^2 ,$$

where the primes denote derivatives. We sketch a proof for the first relation,

$$P_N(1) = \sum_{n=0}^{L(N)} p_n^{(N)} = (N!)^2 , \tag{19}$$

the others may be proven in a similar way. All terms with $n > 1$ in recursion formula (7) contain at least one factor $(1 - y^j)^3$ and thus vanish for $y = 1$. Hence

$$P_N(1) = \frac{1}{N} \frac{(1 - y^N)^3}{(1 - y)^3} P_{N-1}(y) \Big|_{y=1} \tag{20}$$

$$= \frac{1}{N} (1 + y + y^2 + \cdots + y^{N-1})^3 P_{N-1}(y) \Big|_{y=1}$$

$$= N^2 P_{N-1}(1)$$

The relation (19) then follows by $P_1(1) = 1$ and induction.

Introducing a quasi-statistical notation

$$\langle\langle f(n) \rangle\rangle := \frac{1}{(N!)^2} \sum_{n=0}^{L(N)} p_n^{(N)} f(n) \tag{21}$$

we can summarize these results as

$$\mu := \langle\langle n \rangle\rangle = \frac{3}{4} N(N - 1) \tag{22}$$

$$\sigma^2 := \langle\langle n^2 \rangle\rangle - \mu^2 = \frac{1}{24}(2N + 5)N(N - 1)$$

$$\mu_3 := \langle\langle (n - \mu)^3 \rangle\rangle = -\frac{3}{8} N(N - 1) \,.$$

The last result is remarkable since it implies that the "skewness" of the distribution of the $p_n^{(N)}$, defined by [12]

$$\gamma = \frac{\mu_3}{\sigma^3} \tag{23}$$

is asymptotically proportional to $N^{-5/2}$ and thus vanishes for $N \to \infty$. This is compatible with the observation that for large N the distribution of coefficients can be approximated by a symmetric bell-shaped function.

Acknowledgments

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